Density of Energy States and Fermi Energy

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Topics to be covered

- Preliminary idea of energy in 3D box and Fermi distribution function
- Introduction
- Derivation of Density of Energy states
- Derivation of Expression of Fermi Energy
- Mean energy of electron gas at absolute zero
- References

Objectives

- Explain and Derive of Density of energy states
- Derive Expression of Fermi Energy and apply it for solving problems
- Derive Mean energy of electron gas at absolute zero and apply it for solving problems

Prerequisite/Recapitulations

Course Code : BBS01T10

1. The allowed energy for 1D potential box, $E_n = \frac{h^2 n^2}{8mL^2}$

where m is mass of particle, L is the length of potential box and n are positive integers like 1, 2, 3, 4, 5....

The allowed energy for 3D cubical potential box

$$E = \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad \text{-----------(1)}$$

where n_x, n_y and n_z are three quantum numbers which are only positive integer value.

where $n^2 = n_x^2 + n_y^2 + n_z^2$ -------------(2)

$$E = \frac{h^2}{8mL^2} n^2$$

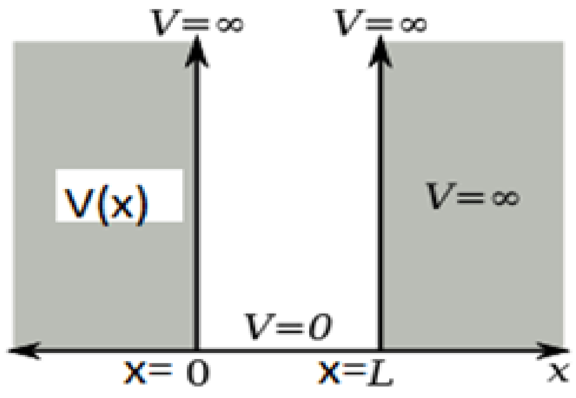
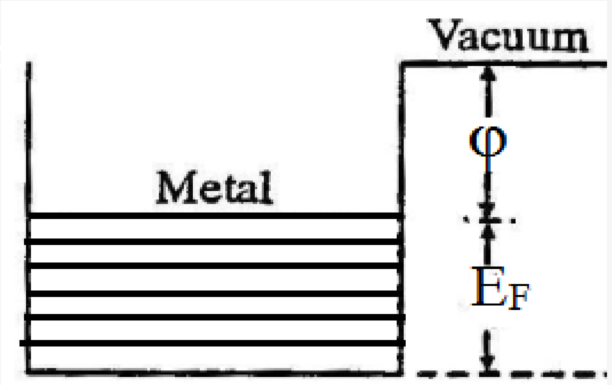


Figure-1

The potential energy within the 1D crystal or box is

$V(x) = 0$ for $0 < x < L$

$V(x) = \infty$ for $x \le 0$ and $x \ge L$



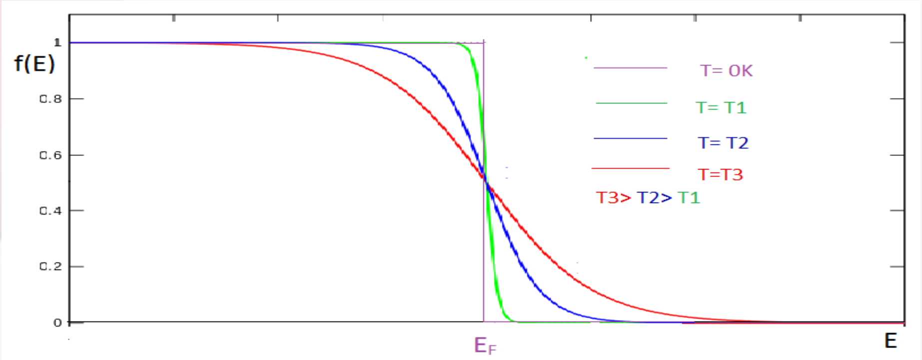
2. The Fermi-Dirac Distribution: The Fermi-Dirac distribution applies to Fermions

- particles with half-integer spin
- obey the Pauli Exclusion Principle.

The Fermi-Dirac Distribution $$f(E) = \frac{1}{1 + \exp[(E - E_F)/k_B T)}$$

f(E) the probability for the occupation of a particular energy level E by an electron then

where k_B is Boltzmann's constant, T is the absolute temperature, E is the energy of the particular energy level E, and E_F is the Fermi energy, the energy of the highest filled level at absolute zero.



At T = 0K,

For E < E_F, $f(E) = \frac{1}{1+e^{-\infty}} = \frac{1}{1+0} = 1$ and **for E > E_F,** $f(E) = \frac{1}{1+e^{\infty}} = \frac{1}{1+\infty} = 0$

Introduction

- Density of energy states is defined by the number of allowed energy states present in unit volume at a given energy.

- Since even at highest energy, the difference between neighbouring energy levels is as small as 10^{-6} eV, in a macroscopically small energy interval dE there are still many discrete energy levels. So the concept of density of energy states is introduced.

- The Fermi energy, E_F is the energy of the highest filled level at absolute zero.

Density of Energy States

•Number of energy states with a particular value of E, depends on the how many combinations of the quantum number (n_x , n_y , n_z) result in the same value n. [From equation (1) $E = \frac{h^2}{8mL^2}\left(n_x^{\ 2} + n_y^{\ 2} + n_z^{\ 2}\right)$]

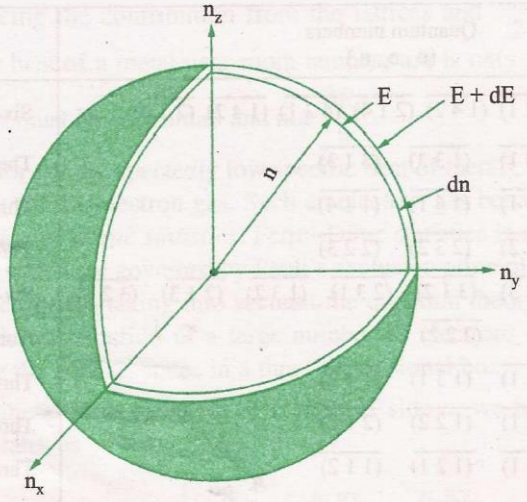


Fig. 1 Density of energy states calculation

•A space of points is constructed with the values of n_x , n_y , n_z

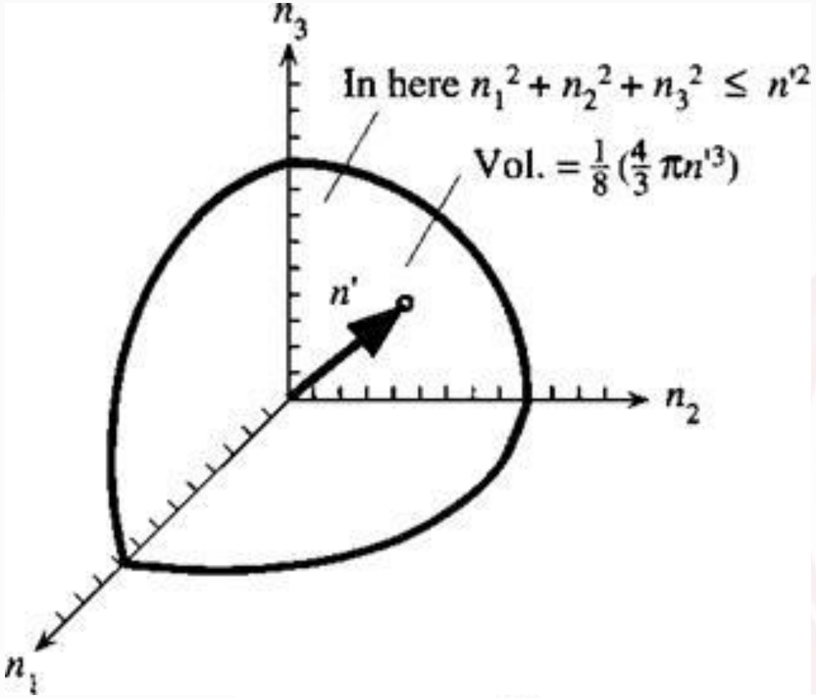
• Each point (n_x , n_y , n_z) with positive integer values of coordinates represents an energy state.

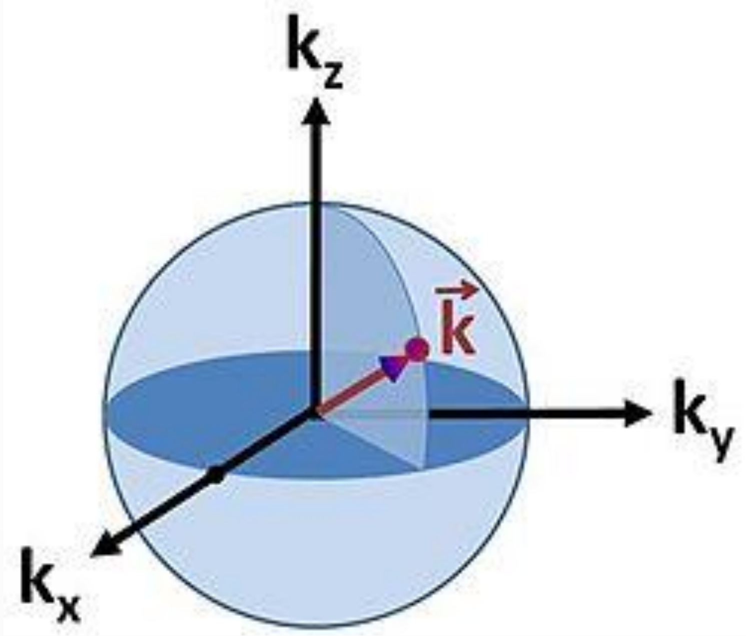
•A radius vector n from the origin is drawn to a point n_x , n_y , n_z in this space and according to equation (2) [$n^2 = n_x^{\ 2} + n_y^{\ 2} + n_z^{\ 2}$] all points on the surface of a sphere of radius n will have the same energy.

• n represents a vector to a point n_x , n_y , n_z in three-dimensional space.

•In this space every integer specifies a state, that is a unit cube contains exactly one state.

• The number of states in any volume is just equal to the numerical value of the volume expressed in units of cubes of lattice parameters.





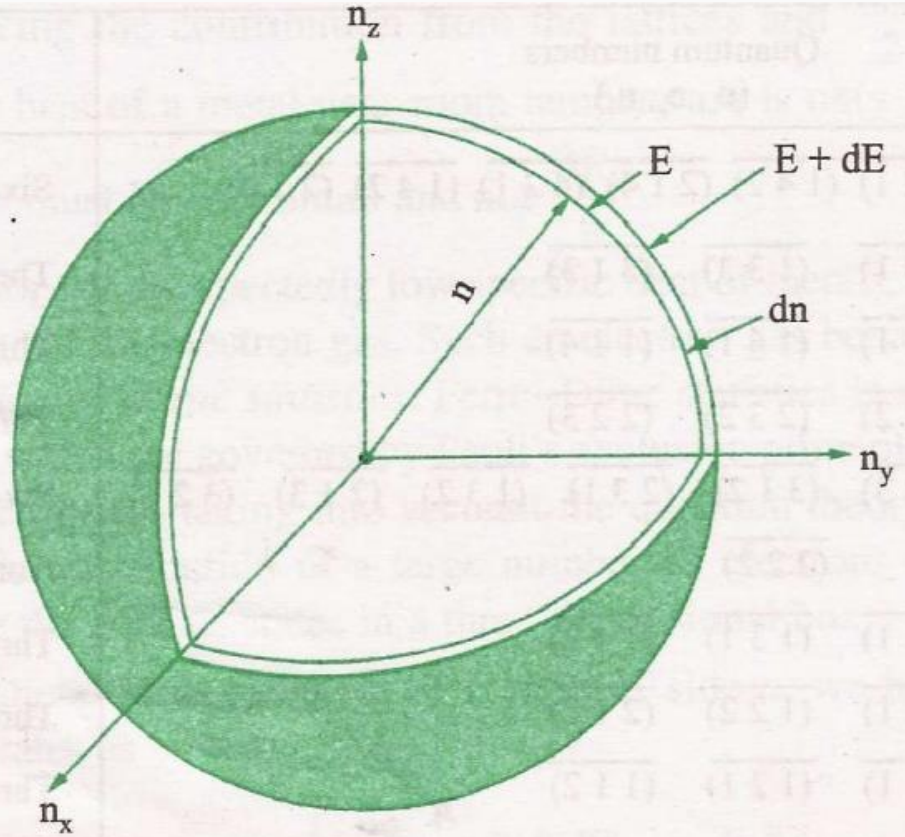


Fig. 1 Density of energy states calculation

Density of Energy States

Number of available states within a sphere of radius n= $\frac{1}{8}\left(\frac{4}{3}\pi n^3\right)$

Number of available states within a sphere of radius (n+dn) =

$$\frac{1}{8}\left[\frac{4}{3}\pi(n+dn)^3\right]$$

The factor 1/8 accounts for the fact that only positive integers are allowable and thus only one octant of the sphere alone be considered.

Number of available states within n to (n+dn) = $\frac{1}{8}\,\frac{4}{3}\pi\left[(n+dn)^3 - n^3\right]$

$$\cong \frac{\pi}{6}\left(3n^2 dn\right)$$

[Neglecting higher order terms of dn]

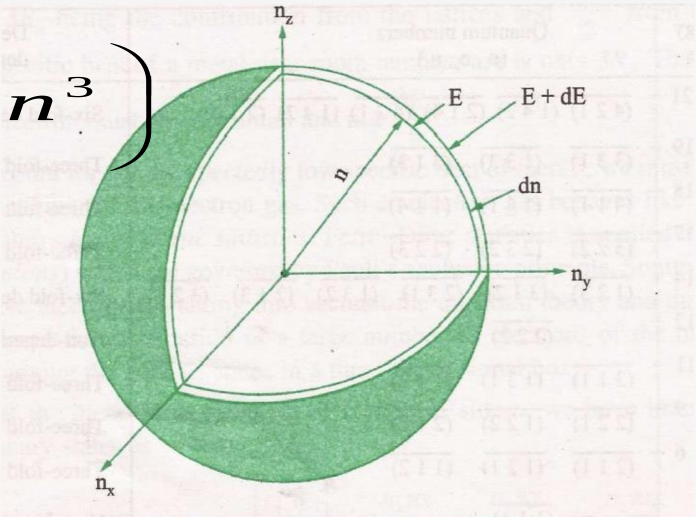


Fig. 1 Density of energy states calculation

Density of Energy States

Number of available states within n to (n+dn) $= \frac{\pi}{2} n^2 dn = \frac{\pi}{4} n\,(2n\,dn)$

From Equation (1), $n^2 = \frac{8mL^2}{h^2} E$ $\quad n = \left[\frac{8mL^2}{h^2}\right]^{1/2} E^{1/2}$

$$2n\ dn = \left[\frac{8mL^2}{h^2}\right] dE$$

Number of available states within E to (E+dE) ,

Z'(E) dE = $\frac{\pi}{4}\left[\frac{8mL^2}{h^2}\right]^{1/2} E^{1/2} \left[\frac{8mL^2}{h^2}\right] dE$

Z'(E) dE = $\frac{\pi}{4}\left[\frac{8mL^2}{h^2}\right]^{3/2} E^{1/2}\ dE$

Density of Energy States

It should be remembered that the Pauli's exclusion principle permits two electrons in each state, so that the number of energy levels actually available are

$$Z'(E)\,dE = 2\,\frac{\pi}{4}\left[\frac{8mL^2}{h^2}\right]^{3/2} E^{1/2}\,dE$$

$$Z'(E)\,dE = \frac{\pi}{2}\left[\frac{8mL^2}{h^2}\right]^{3/2} E^{1/2}\,dE \text{ ---(4)}$$

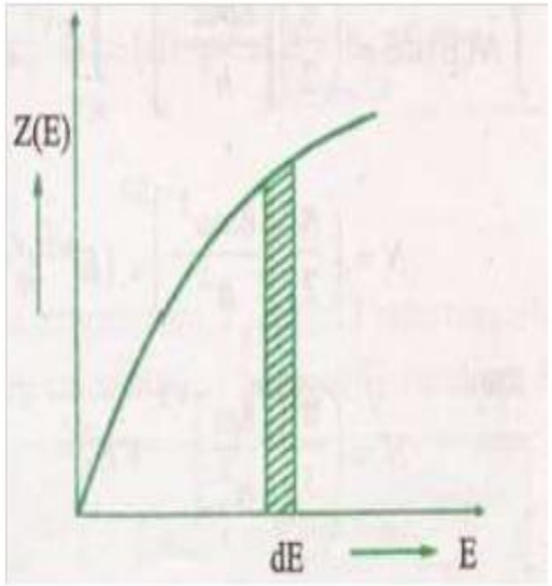


Fig 2: Density of states as a function of electron energy

Density of energy states having energy values lying between E and E+dE,

$$Z(E)\,dE = Z'(E)\,dE/V = \frac{\pi}{2}\left[\frac{8m}{h^2}\right]^{3/2} E^{1/2}\,dE \quad , \quad [\text{As } L^3 = V]$$

Expression of Fermi Energy

Number of electrons in a system that have energy E to E+dE is N(E) dE = Z(E) dE F(E) where F(E) is the Fermi function

$$N(E)dE = \frac{\pi}{2}\left[\frac{8m}{h^2}\right]^{3/2} V\,E^{1/2}dE\,\frac{1}{1+e^{\frac{E-E_F}{kT}}}$$ (Using eqn (4))

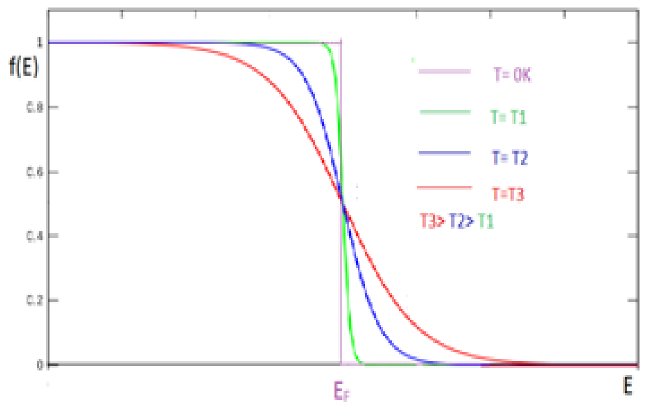


Figure-3

Total number of electrons, N = ∫ N(E)dE

- At absolute zero, the distribution f(E) is simple and all states up to Fermi level are filled and those above E_F are empty.

For T=0K, f(E) =0 for E>E_F and f(E) = 1 for E<E_F

Total number of electrons, N = ∫ N(E)dE $= \frac{\pi}{2}\left[\frac{8m}{h^2}\right]^{3/2} V\int_0^{E_F} E^{1/2}\, dE$

Expression of Fermi Energy

Total number of electrons, N = $\int N(E)\, dE$

$$N = \frac{\pi}{3}\left[\frac{8m}{h^2}\right]^{3/2} V\, E_F^{3/2}$$

Number of electrons per unit volume= density of electrons,

$$n = \frac{N}{V} = \frac{\pi}{3}\left[\frac{8m}{h^2}\right]^{3/2} E_F^{3/2}$$

$$E_F = \frac{h^2}{8m}\left[\frac{3n}{\pi}\right]^{2/3}$$

$= 0.58 \times 10^{-37}\, n^{2/3}$ Joule

The value of E_F gives the top most energy level at absolute zero.

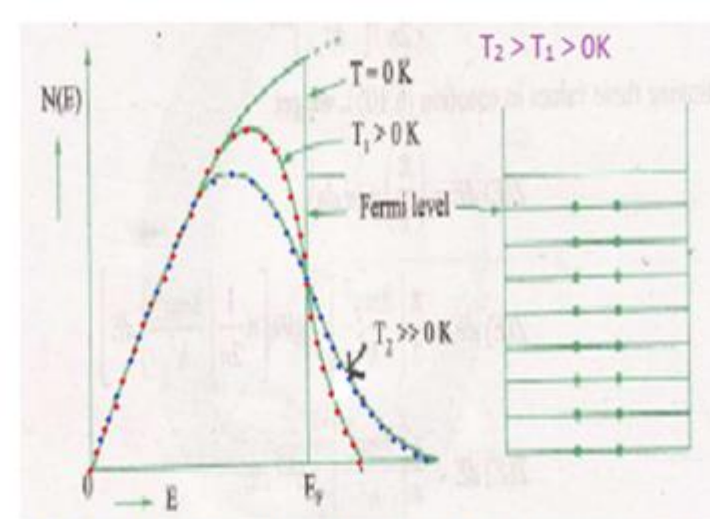


Fig: 5 The Population Density of a free electron gas

Mean Energy of Electron Gas at absolute Temperature zero

Mean Energy of electron at 0K is $\overline{E}_0 = \dfrac{Total\ energy\ at\ 0K\ (U_0)}{Total\ number\ of\ electrons\ (N)}$

$$U_0 = \int_0^{E_F} Z(E)\,dE\ f(E)\,E \quad where\ f(E) = 1 \quad for\ 0 < E < E_F$$

$$U_0 = \frac{\pi}{2}\left[\frac{8mL^2}{h^2}\right]^{3/2} \int_0^{E_F} E^{3/2}\,dE\ , \quad [Using\ eqn\ (5)] \qquad U_0 = \frac{\pi}{5}\left[\frac{8mL^2}{h^2}\right]^{3/2} E_F^{\ 5/2}$$

$$\overline{E}_0 = \frac{U_0}{N} = \frac{\frac{\pi}{5}E_F^{5/2}}{\frac{\pi}{3}E_F^{3/2}}$$

$$\overline{E}_0 = \frac{3}{5}E_F \quad where\ \ E_F = \left(\frac{h^2}{8m}\right)\left[\frac{3n}{8\pi}\right]^{2/3}$$

Practice Questions

1. Define density of energy states and derive its expression.
2. Define Fermi Energy. Derive its expression.
3. Calculate the Fermi Energy for sodium. Given Atomic weight is 23gm/mole, density of sodium 0.971gm/cm^3 (Assume one free electron/atom)
4. If the Fermi energy is 10eV, what is the mean energy of electron at 0K.

References

1. J. Singh , Semiconductor optoelectronics, Physics and Technology, Mc-Graw –Hill Inc. 1995.
2. S.M. Sze, Semiconductor Devices: Physics and Technology, Wiley 2008.
3. Pillai S O, Solid State Physics,(2010), sixth edition, New Age International (P) Ltd. ISBN-9788122427264.
4. https://www.youtube.com/watch?v=tFSZUHRQa3k
5. https://www.youtube.com/watch?v=z7YGS67GETo&t=216s5.

Thank you